

Print selected from Online session

d his

(FILE 'HOME' ENTERED AT 13:29:46 ON 08 SEP 2004)

FILE 'REGISTRY' ENTERED AT 13:30:01 ON 08 SEP 2004

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 0 S L2
L4 2 S L2 FULL
L5 0 S L2 CSS FULL
L6 STRUCTURE UPLOADED
L7 0 S L6
L8 10 S L6 FULL

FILE 'CAPLUS' ENTERED AT 13:34:51 ON 08 SEP 2004

L9 2 S L4
L10 1 S L8

FILE 'CASREACT' ENTERED AT 13:41:18 ON 08 SEP 2004

L11 STRUCTURE UPLOADED
L12 0 S L11
L13 0 S L11 FULL

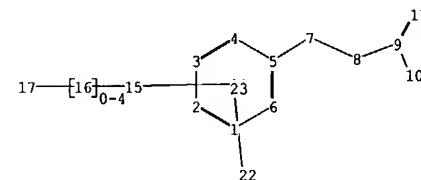
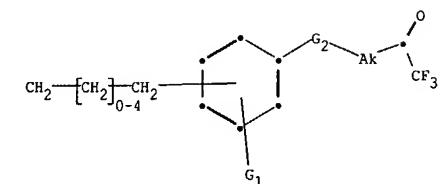
FILE 'CAPLUS' ENTERED AT 13:42:06 ON 08 SEP 2004

L14 10 S ?TRIFLUOROPENTANONE OR ?TRIFLUOROOCTANONE OR ?TRIFLUORODODECA
L15 3 S L14 AND (PHENYL? OR PHENOXY? OR BENZYL?)
L16 1 S L10 AND (TREAT? OR PREVENT? OR INHIBIT? OR OBESITY OR METABOL
L17 13607 S ?HEXADECANOIC ACID?
L18 387 S L17 AND ?LACTONE?
L19 1 S L18 AND ACETIC ANHYDRIDE
L20 3 S L18 AND TRIFLUOROMETHYL?

FILE 'BIOSIS' ENTERED AT 13:50:19 ON 08 SEP 2004

L21 378785 S OBESITY OR METABOLIC DISORDER? OR HYPOTENSION OR DIABETES OR
L22 110858 S L21 AND (TREAT? OR PREVENT? OR INHIBIT?)
L23 975 S L22 AND LIPASE
L24 1 S L23 AND ?TRIFLUORO?

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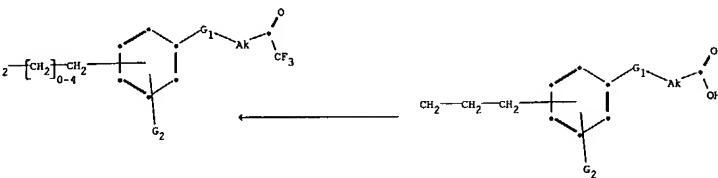


chain nodes :
 7 8 9 10 11 12 13 15 16 17 22
 ring nodes :
 1 2 3 4 5 6
 chain bonds :
 5-7 7-8 8-9 9-10 9-11 12-13 15-16 16-17
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 exact/norm bonds :
 5-7 7-8 8-9 9-11 12-13
 exact bonds :
 9-10 15-16 16-17
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 isolated ring systems :
 containing 1 :

G1:H,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,X,Ak

G2:O,Ak,[*1]

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:CLASS 20:CLASS 22:CLASS 23:CLASS
 Element Count :
 Node 8: Limited
 C,C1-15



main nodes :
 7 8 9 10 11 12 13 14 15 16 18 33 34 35 36 37 38 39 40 41 42 44
 ring nodes :
 1 2 3 4 5 6 27 28 29 30 31 32
 main bonds :
 5-7 7-8 8-9 9-10 9-11 12-13 14-15 15-16 31-33 33-34 34-35 35-36 35-37 38-39
 40-41 41-42
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 27-28 27-32 28-29 29-30 30-31 31-32
 exact/norm bonds :
 5-7 7-8 8-9 9-11 12-13 31-33 33-34 34-35 38-39
 exact bonds :
 9-10 14-15 15-16 40-41 41-42
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 27-28 27-32 28-29 29-30 30-31 31-32 35-36 35-37
 isolated ring systems :
 containing 1 : 27 :

1:0,[*1]

2:H,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,X,Ak

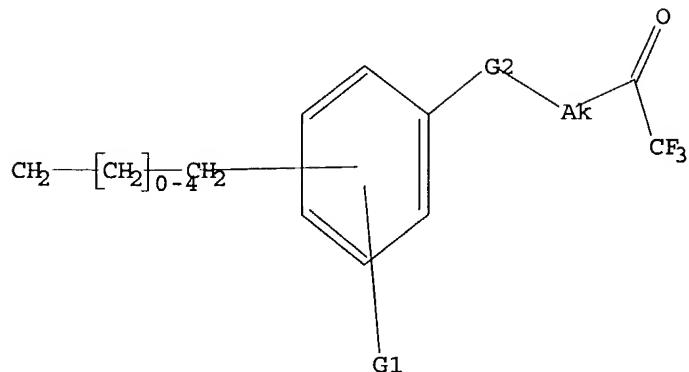
catch level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:CLASS 34:CLASS 35:CLASS
 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS
 45:CLASS

fragments assigned product role:
 containing 1
 fragments assigned reactant/reagent role:
 containing 27

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L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



O
||
1
G1 H, MeO, EtO, n-PrO, i-PrO, n-BuO, i-BuO, X, Ak
G2 O, Ak, [@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l1
GENERIC GROUP NOT VALID HERE
Generic groups may not be used in these circumstances:

1. Any generic group node (e.g., Hy) in a ring.
2. An Ak node attached to another Ak node.

=>
Uploading C:\Program Files\Stnexp\Queries\240.str

L2 STRUCTURE UPLOADED

=> s l2
SAMPLE SEARCH INITIATED 13:32:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4099 TO ITERATE

24.4% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) 0 ANSWERS

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 78141 TO 85819
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

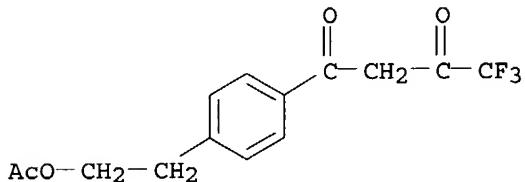
=> s 12 full
FULL SEARCH INITIATED 13:32:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 80927 TO ITERATE

100.0% PROCESSED 80927 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.02

L4 2 SEA SSS FUL L2

=> d scan

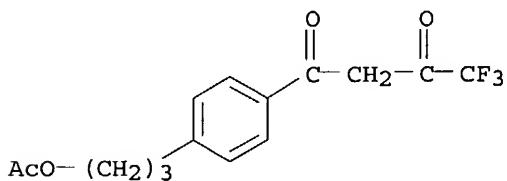
L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1,3-Butanedione, 1-[4-[2-(acetyloxy)ethyl]phenyl]-4,4,4-trifluoro- (9CI)
MF C14 H13 F3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1,3-Butanedione, 1-[4-[3-(acetyloxy)propyl]phenyl]-4,4,4-trifluoro- (9CI)
MF C15 H15 F3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

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Print selected from Online session

=> s 12 css full
FULL SEARCH INITIATED 13:33:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 80927 TO ITERATE

100.0% PROCESSED 80927 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

L5 0 SEA CSS FUL L2

=>
Uploading C:\Program Files\Stnexp\Queries\240.str

L6 STRUCTURE UPLOADED

=> s 16
SAMPLE SEARCH INITIATED 13:34:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3355 TO ITERATE

29.8% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 63627 TO 70573
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> s 16 full
FULL SEARCH INITIATED 13:34:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 66484 TO ITERATE

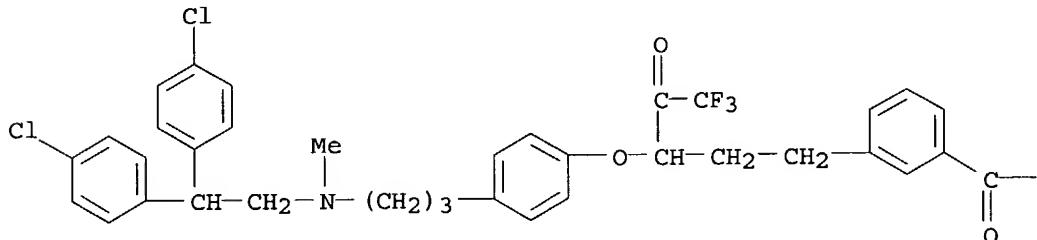
100.0% PROCESSED 66484 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.02

L8 10 SEA SSS FUL L6

=> d scan

L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzoic acid, 3-[3-[4-[3-[(2,2-bis(4-chlorophenyl)ethyl)methylamino]propyl]phenoxy]-5,5,5-trifluoro-4-oxopentyl]-, 1,1-dimethylethyl ester (9CI)
MF C40 H42 Cl2 F3 N O4

PAGE 1-A



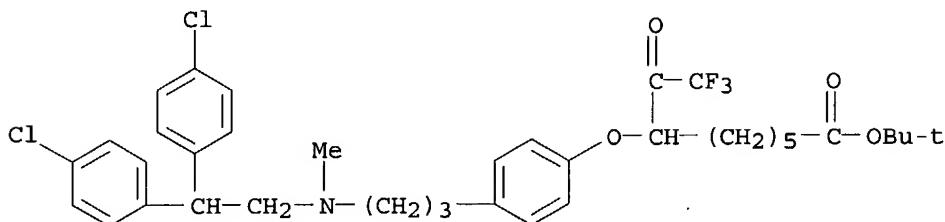
Print selected from Online session

—OBu-t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

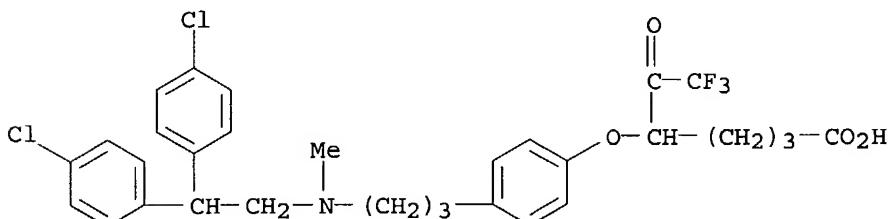
L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Nonanoic acid, 7-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-9,9,9-trifluoro-8-oxo-, 1,1-dimethylethyl ester (9CI)
MF C37 H44 Cl2 F3 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

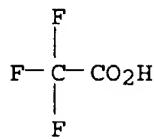
L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Heptanoic acid, 5-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-7,7,7-trifluoro-6-oxo-, trifluoroacetate (9CI)
MF C31 H32 Cl2 F3 N O4 . C2 H F3 O2

CM 1

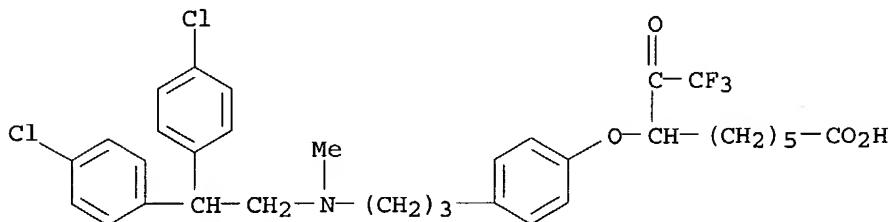


CM 2

Print selected from Online session



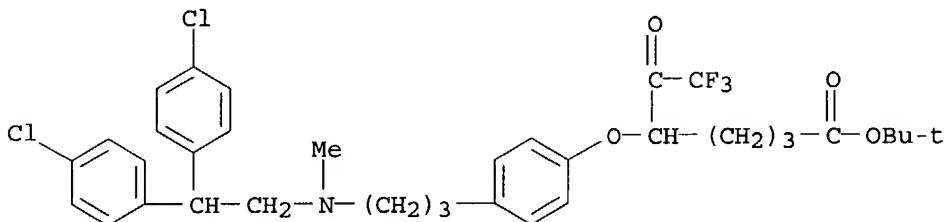
L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Nonanoic acid, 7-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-9,9,9-trifluoro-8-oxo- (9CI)
MF C33 H36 Cl2 F3 N O4
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Heptanoic acid, 5-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-7,7,7-trifluoro-6-oxo-, 1,1-dimethylethyl ester (9CI)
MF C35 H40 Cl2 F3 N O4

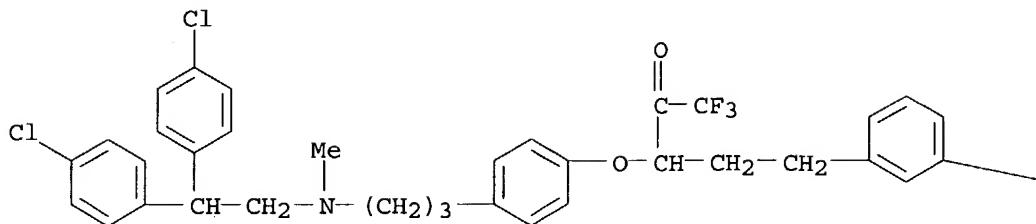


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzoic acid, 3-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-5,5,5-trifluoro-4-oxopentyl]- (9CI)
MF C36 H34 Cl2 F3 N O4
CI COM

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PAGE 1-A



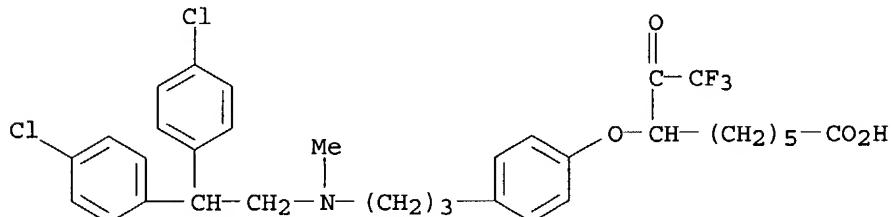
PAGE 1-B

—CO2H

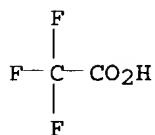
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

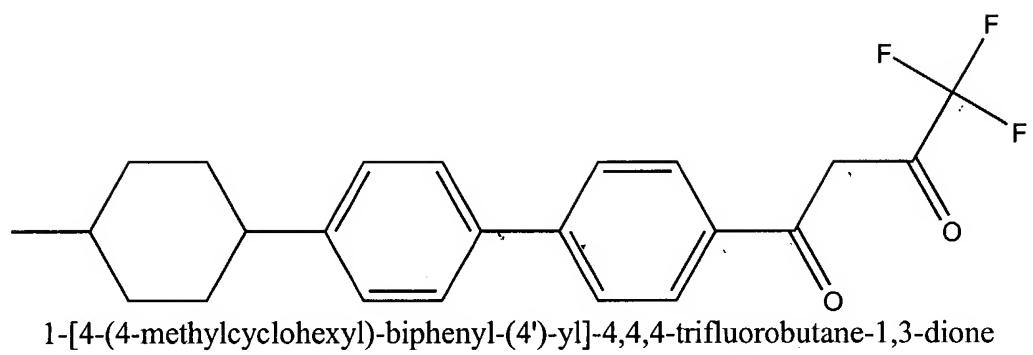
L8 10 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Nonanoic acid, 7-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-9,9,9-trifluoro-8-oxo-, trifluoroacetate (9CI)
MF C33 H36 Cl2 F3 N O4 . C2 H F3 O2

CM 1

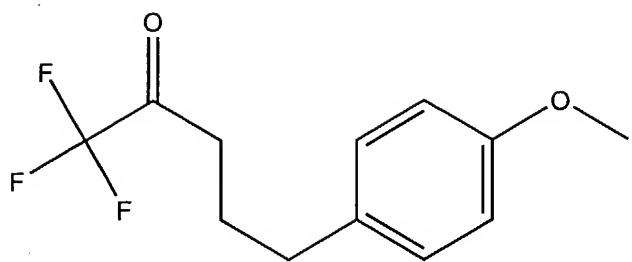


CM 2





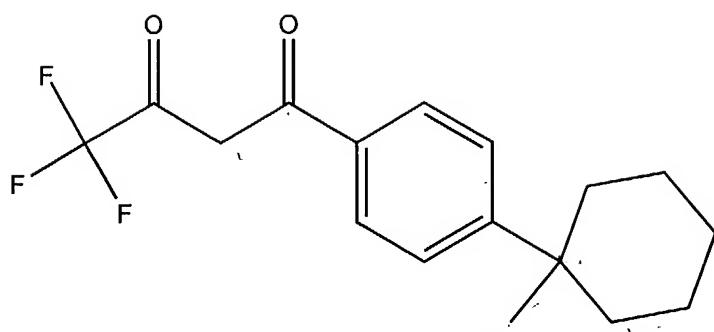
1-[4-(4-methylcyclohexyl)-biphenyl-(4')-yl]-4,4,4-trifluorobutane-1,3-dione



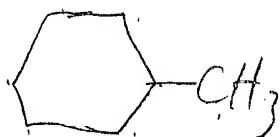
5-(4-methoxyphenyl)-1,1,1-trifluoropentan-2-one

J. org. chem.

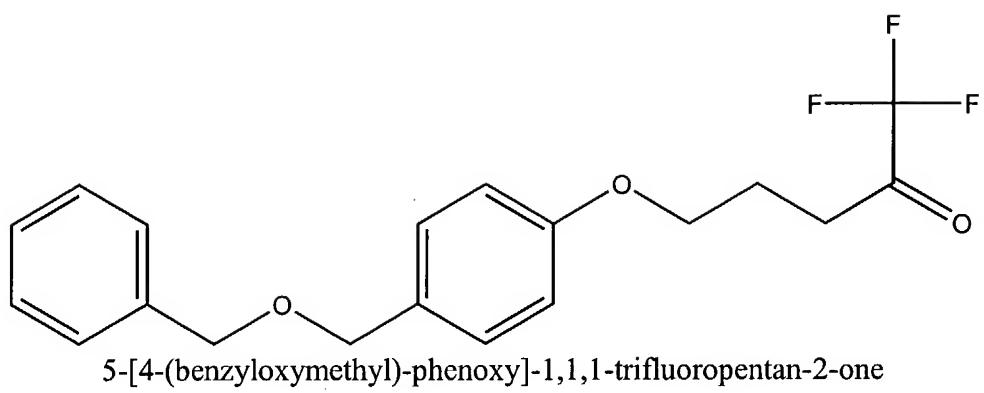
19.88

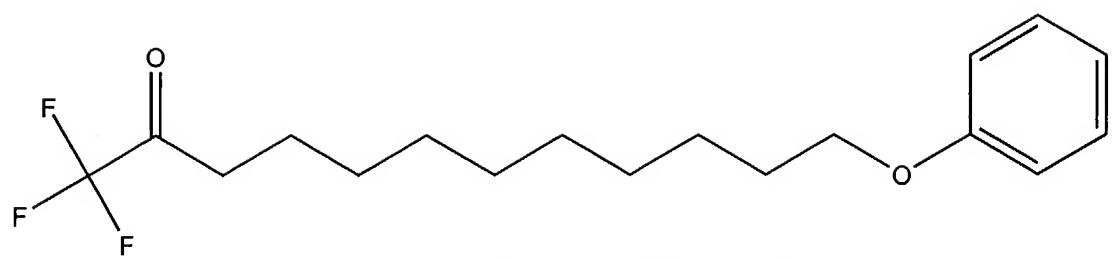


1-[4-(methylcyclohexyl)-phenyl]-4,4,4-trifluorobutane-1,3-dione



19.297.515





1,1,1-trifluoro-12-phenoxy-dodecan-2-one

